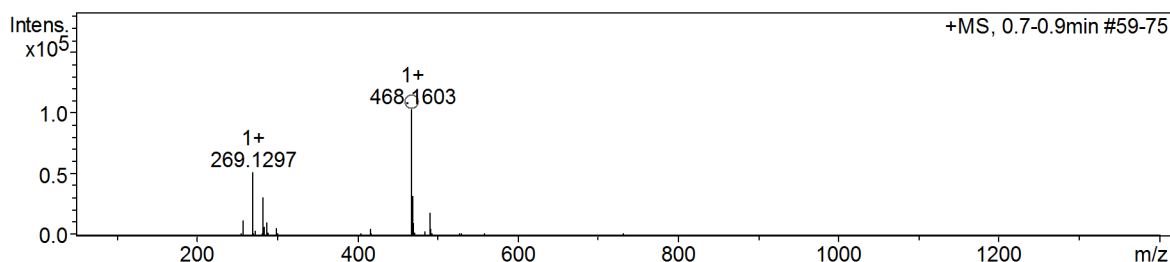




Sample-ID	m_cal_681	Lab	C13
Submitter	Michael Callingham	Supervisor	Hon Lam
Analysis Name	m_cal_681_526330_1_01_23303.d	Acquisition Date	5/18/2016 6:40:09 PM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #59-75



#	m/z	I %
1	255.1141	1.8
2	257.1295	12.0
3	258.1328	2.1
4	269.1297	50.3
5	270.1327	9.1
6	273.1250	3.5
7	283.1453	30.2
8	284.1492	6.7
9	287.1404	10.8
10	288.1440	2.0
11	299.1405	5.7
12	416.1975	5.2
13	468.1603	100.0
14	469.1633	30.8
15	470.1630	9.8
16	471.1638	2.0
17	484.1297	3.1
18	490.1422	17.8
19	491.1448	5.5
20	558.1291	1.8

Generate Molecular Formula Parameters

Charge	Tolerance	sigma limit	H/C Ratio	Electron Conf.	Nitrogen Rule	Chrom.BackGround	Calibration
+1	6 ppm	0.08	3 - 0	both	false	false	TRUE
Expected Formula		C27 H27 N1 O3 S1				Adduct(s):	H, Na, NH4, radical
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	468.1603	468.1604	0.20	0.0009	C27H27NNaO3S	M+Na	22.9898

Note: Sigma fits < 0.05 indicates high probability of correct MF